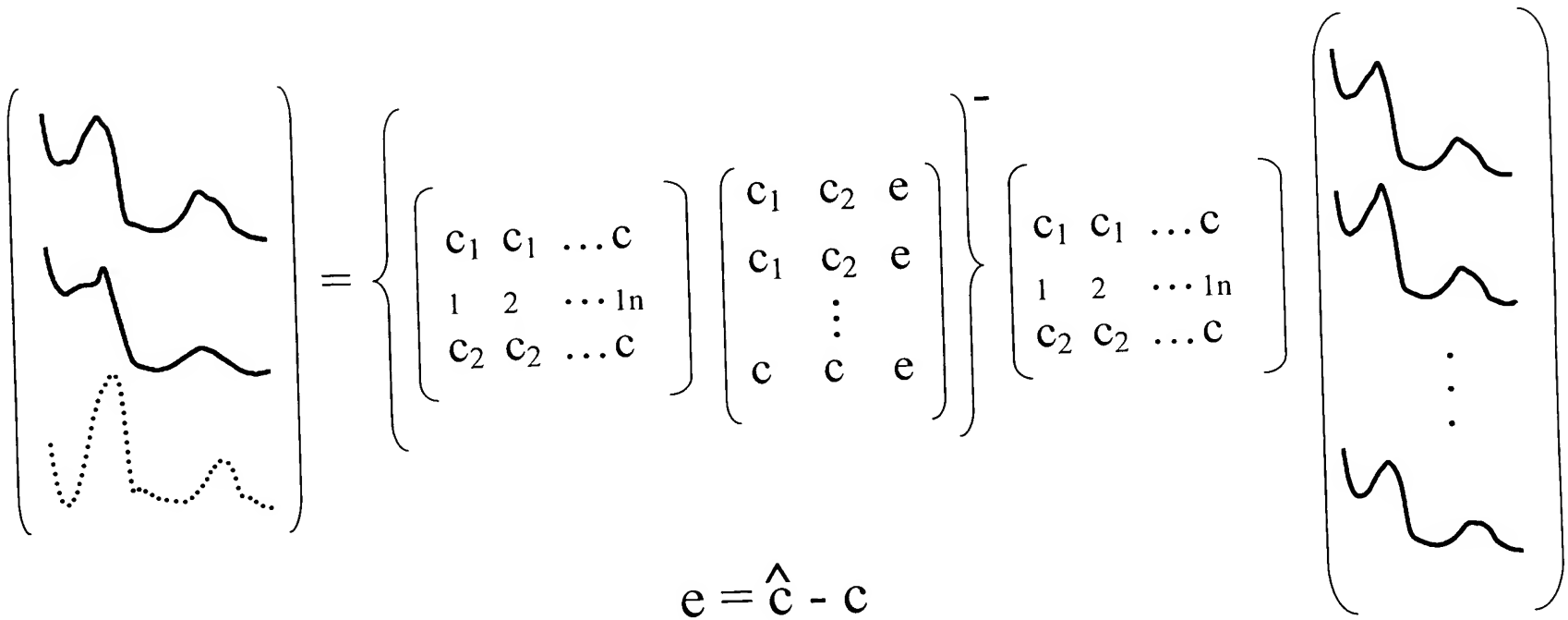
$$\hat{\tilde{K}} = (\tilde{C}^T \tilde{C})^{-1} \tilde{C}^T$$



$$e = \hat{c} - c$$

Fig. 1

$$\tilde{\tilde{\mathbf{C}}} = \mathbf{A}\ \tilde{\tilde{\mathbf{K}}}^{T}\ (\tilde{\tilde{\mathbf{K}}}\ \tilde{\tilde{\mathbf{K}}}^{T})^{-1}$$

$$\begin{pmatrix} \hat{c}_1 & \hat{c}_2 & \hat{c}_e \\ \hat{c}_1 & \hat{c}_2 & \hat{c}_e \\ \vdots & \vdots & \\ \hat{c} & \hat{c} & \hat{c}_e \end{pmatrix} =$$

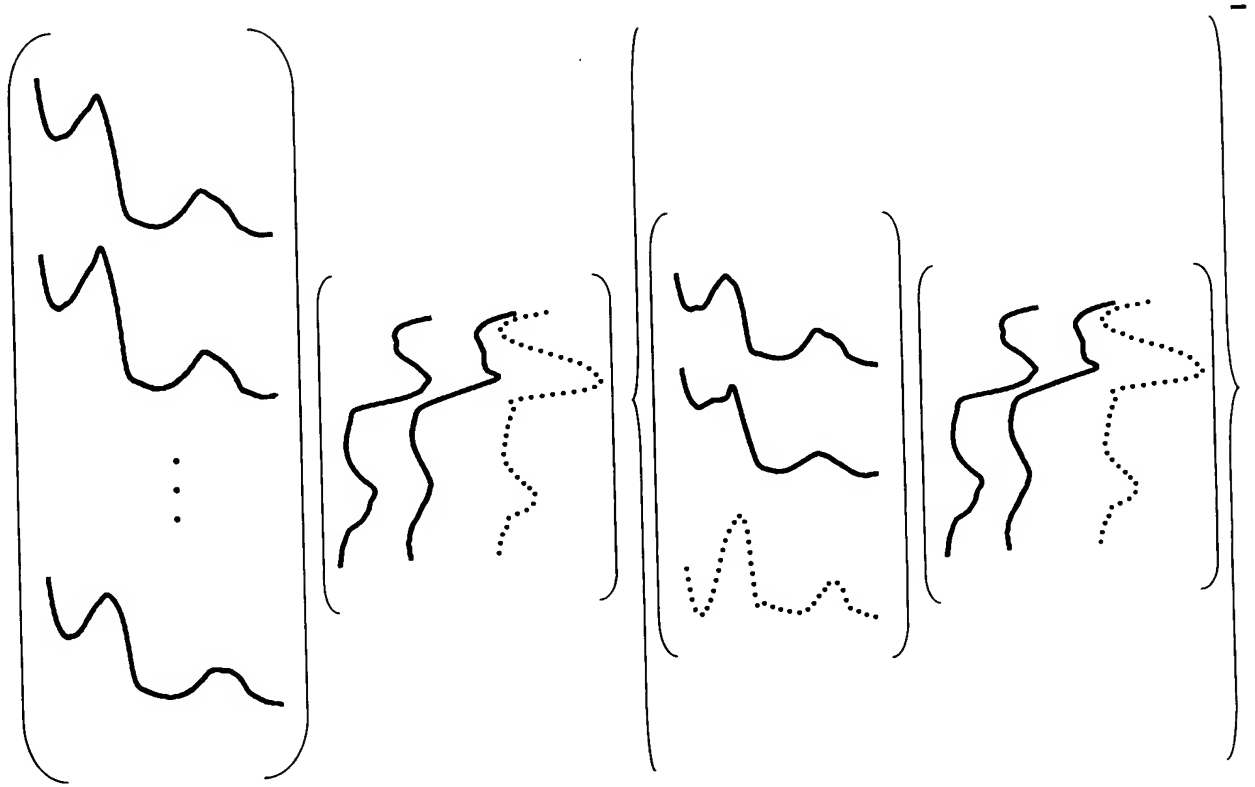


Fig. 2

Spectral-Residual Augmented CLS

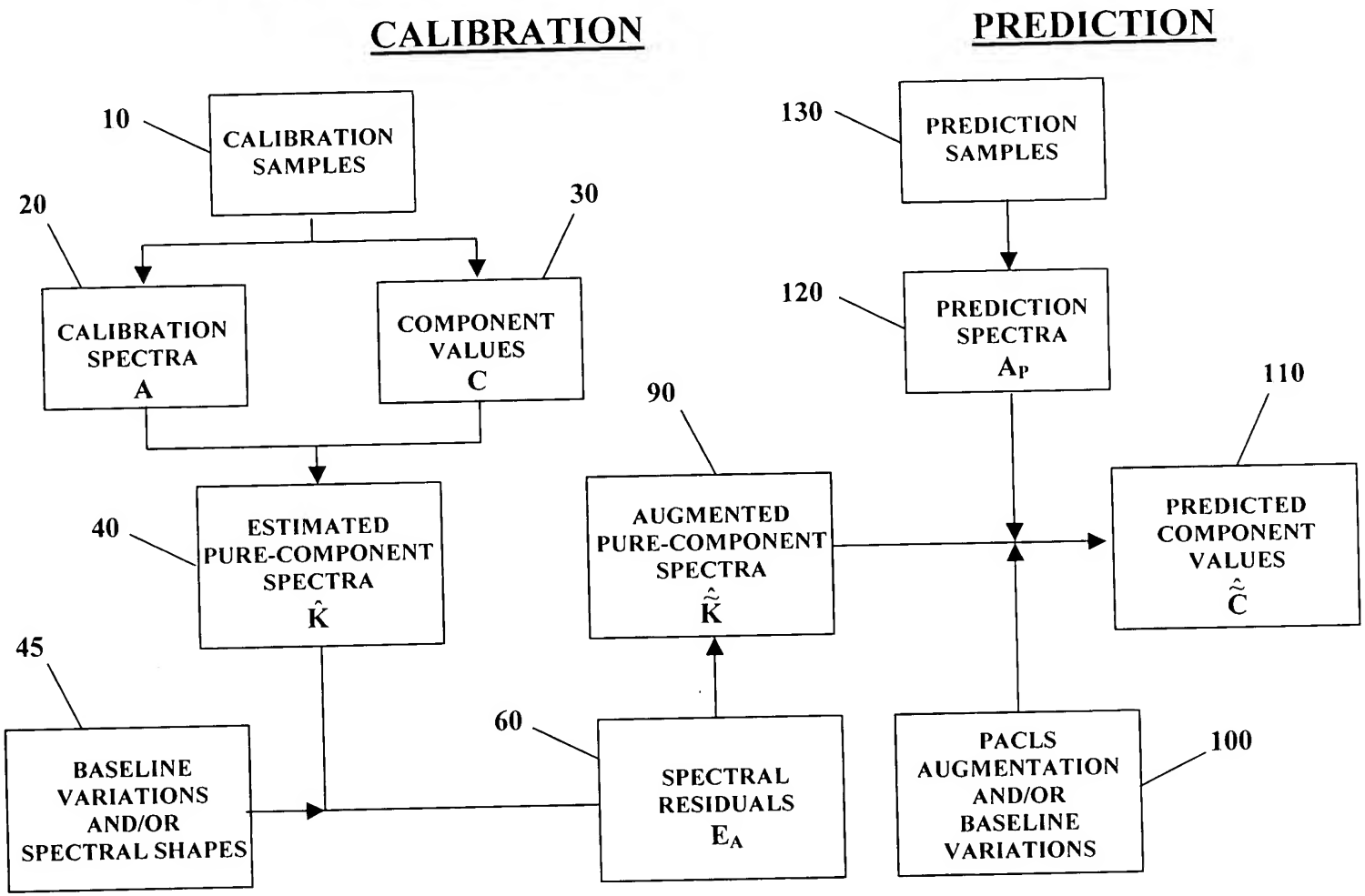


Fig. 3A

Scores Augmented CLS

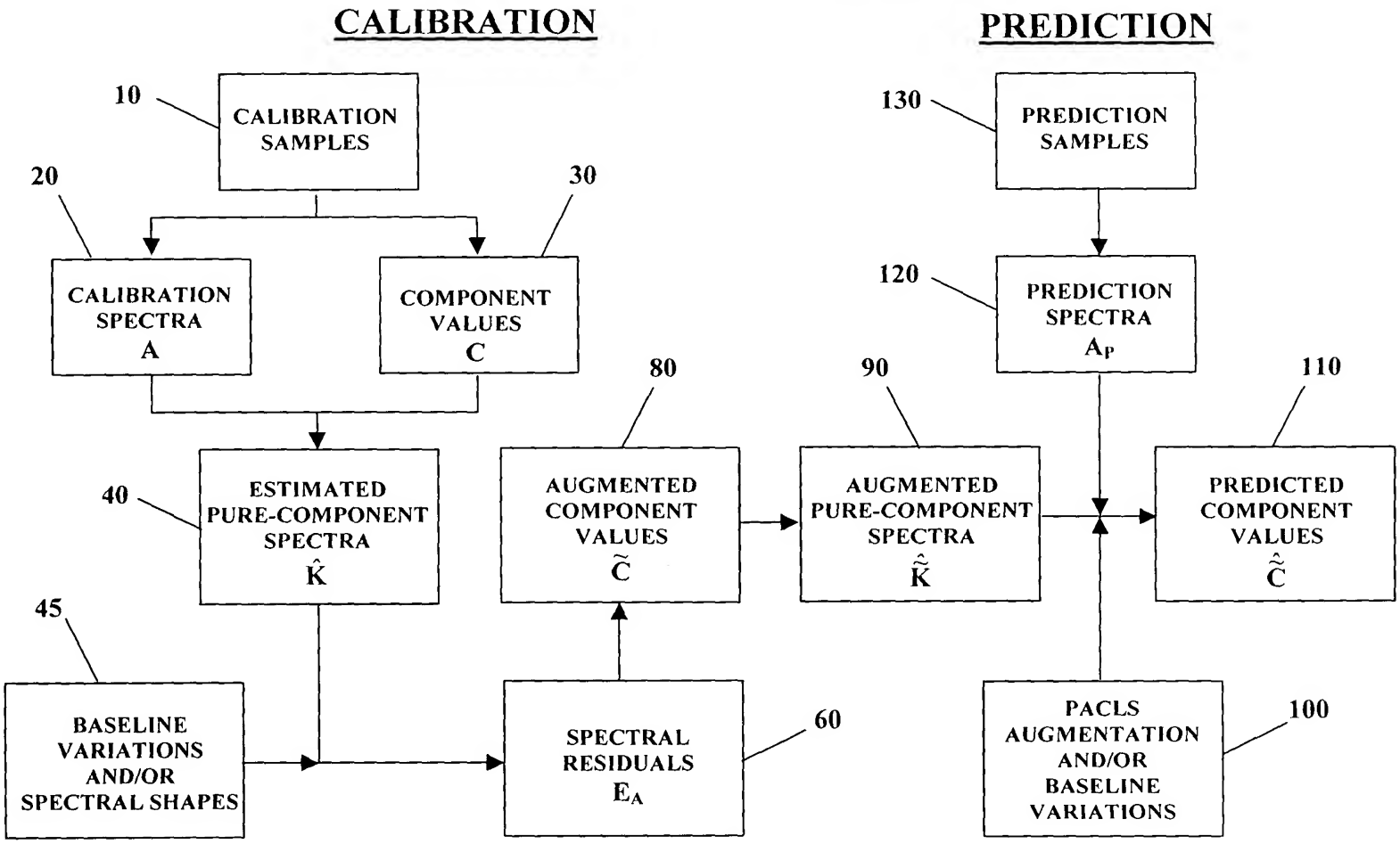


Fig. 3B

Concentration-Residual Augmented CLS

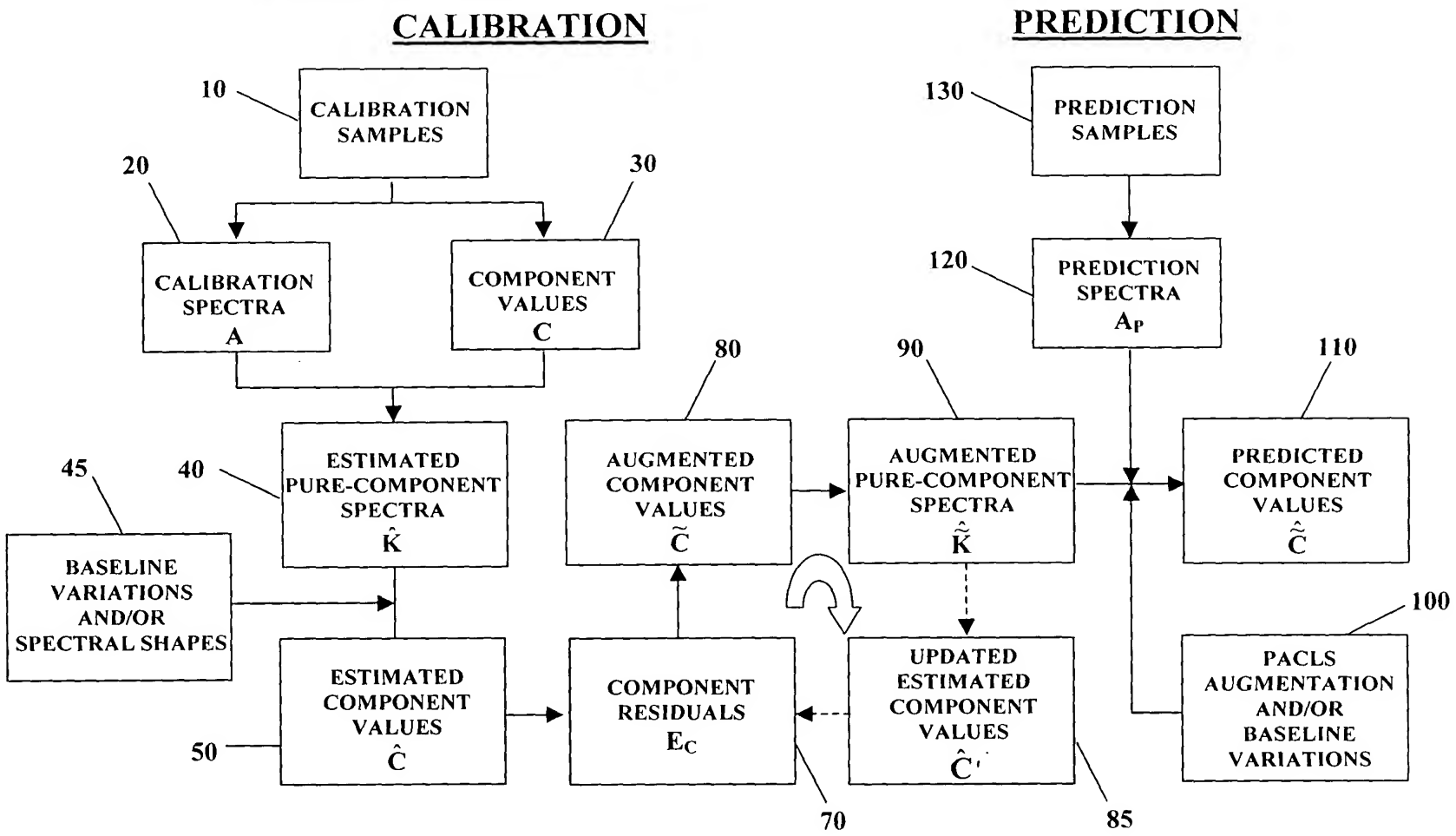


Fig. 4

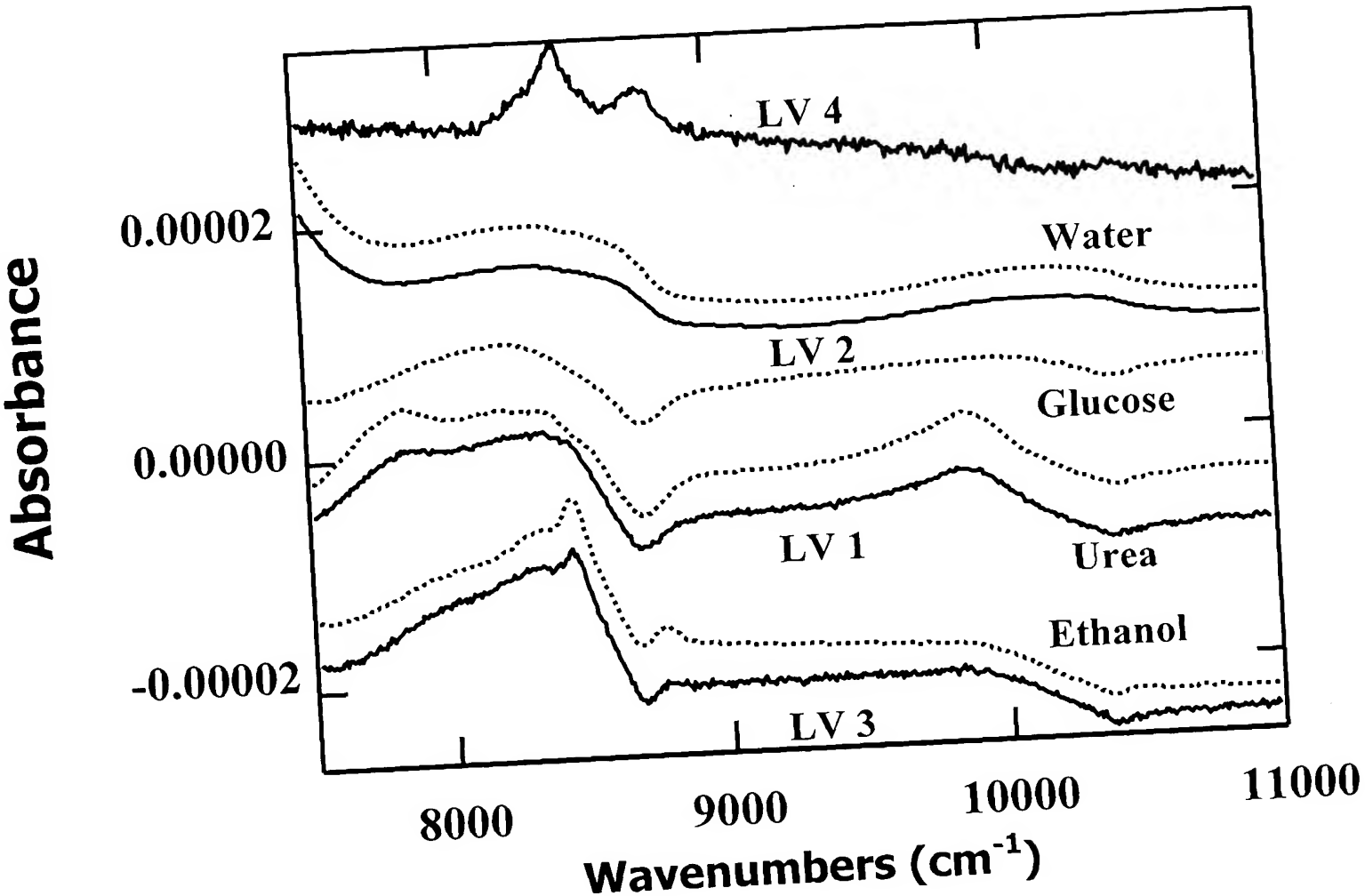

LV 4
Water
LV 2
Glucose
LV 1
Urea
Ethanol
LV 3
0.00002
0.00000
-0.00002
Absorbance
8000
9000
10000
11000
Wavenumbers (cm-1)

Fig. 5

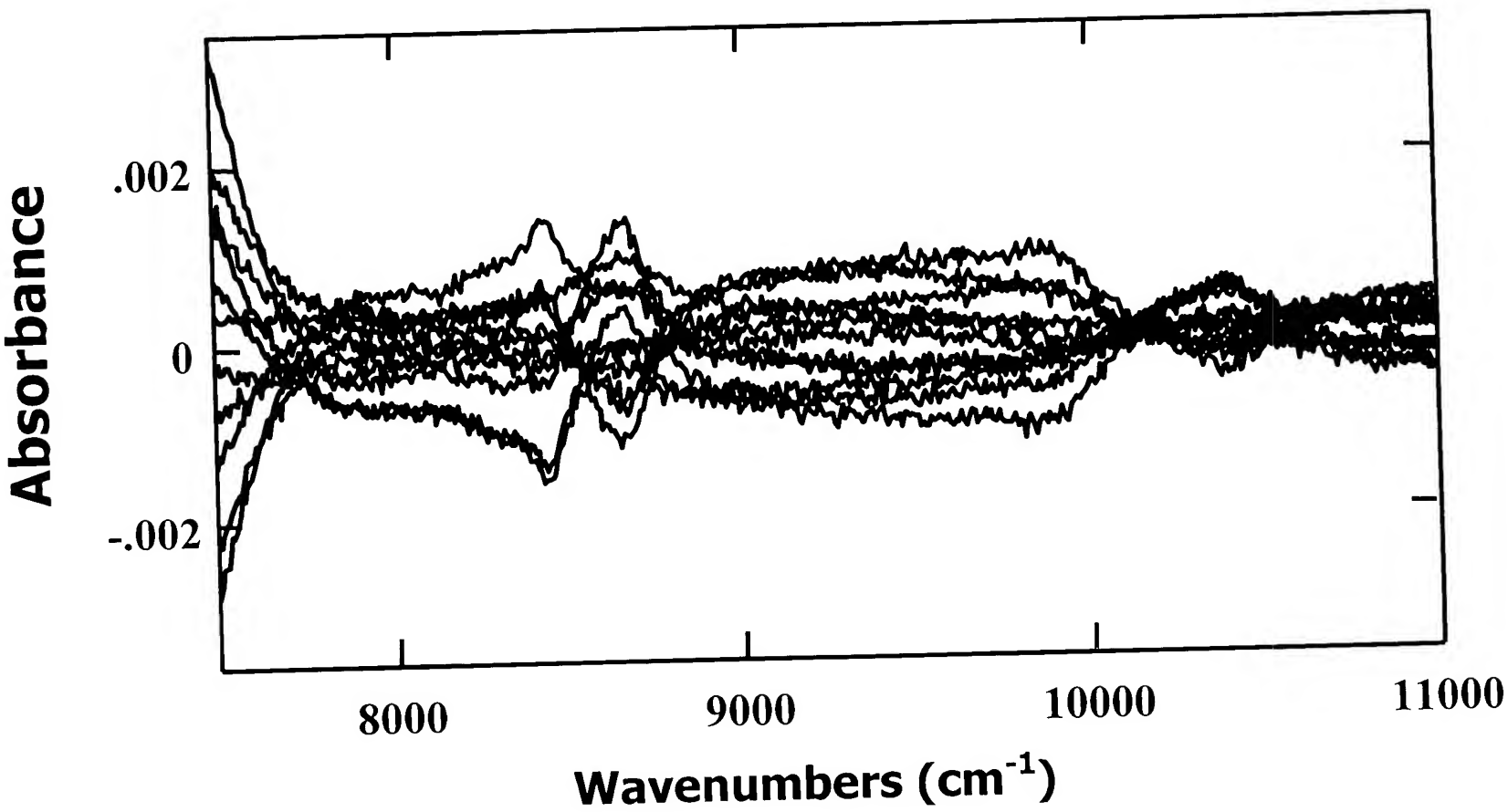


Fig. 6

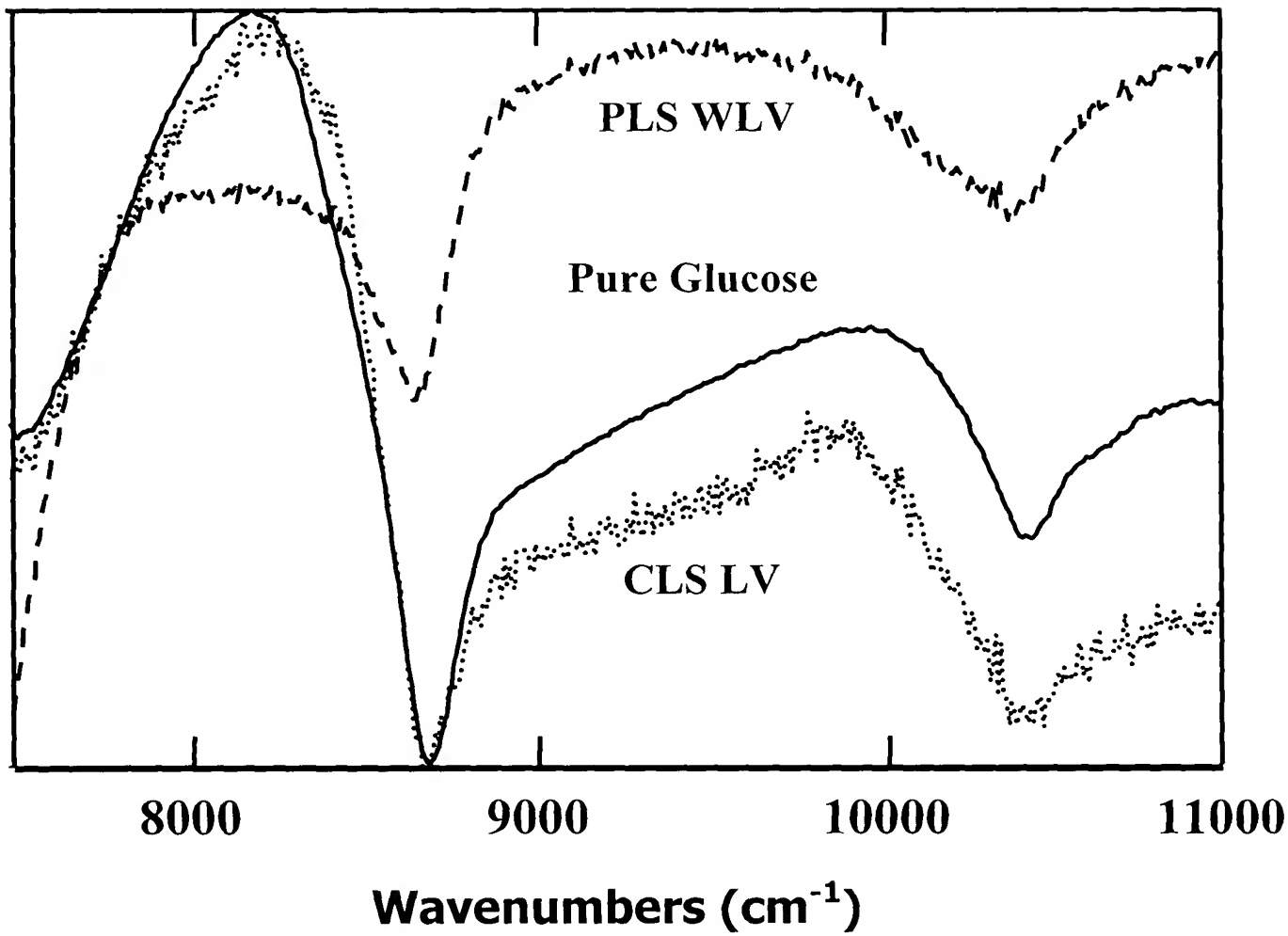

PLS WLV
Pure Glucose
CLS LV
8000
9000
10000
11000
Wavenumbers (cm-1)

Fig. 7

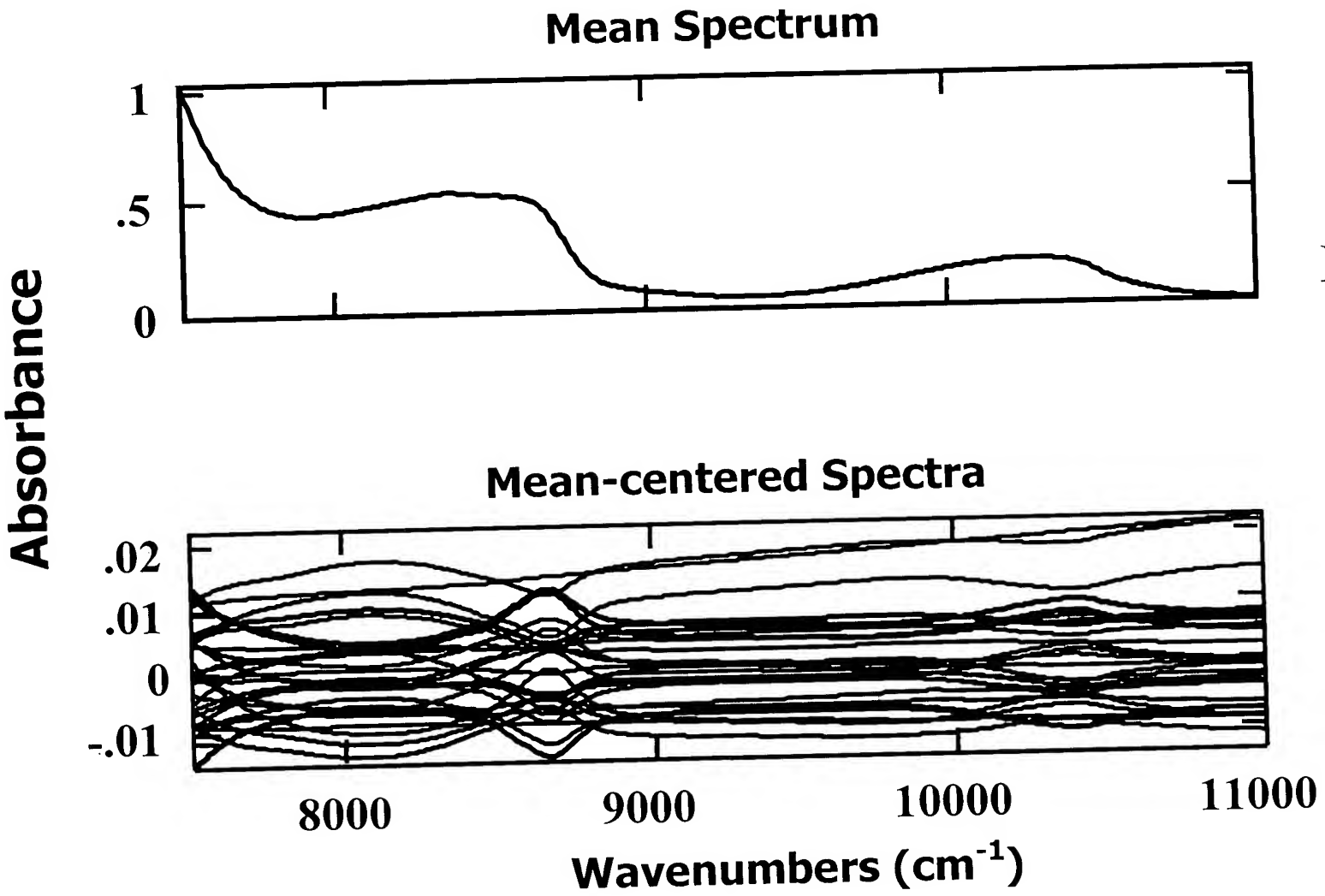

Mean Spectrum
1
.5
0
Absorbance
Mean-centered Spectra
.02
.01
0
-.01
8000
9000
10000
11000
Wavenumbers (cm-1)

Fig. 8A

Fig. 8B

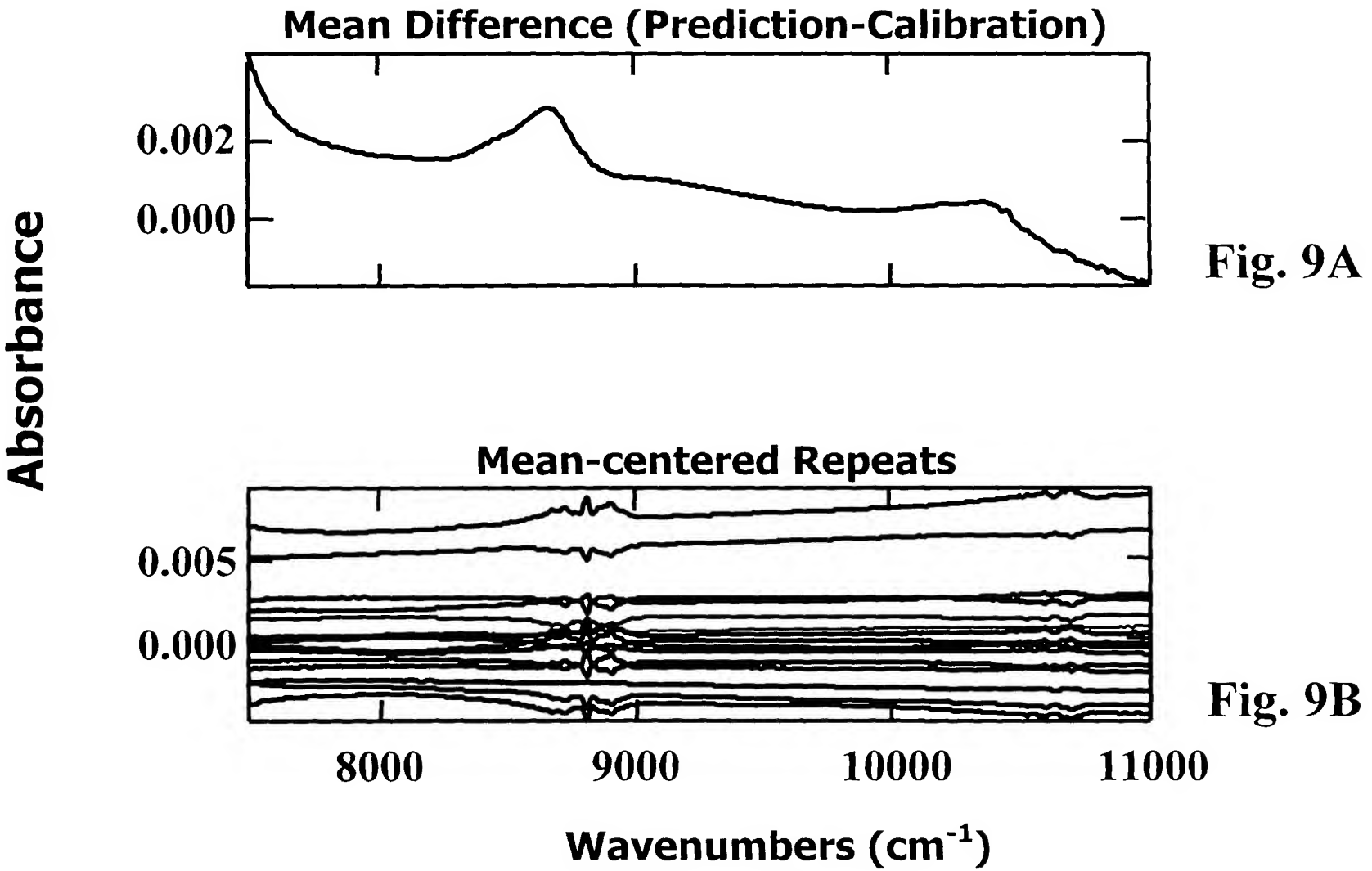

Mean Difference (Prediction-Calibration)
0.002
0.000
Absorbance
Mean-centered Repeats
0.005
0.000
8000
9000
10000
11000
Wavenumbers (cm-1)

Fig. 9A

Fig. 9B

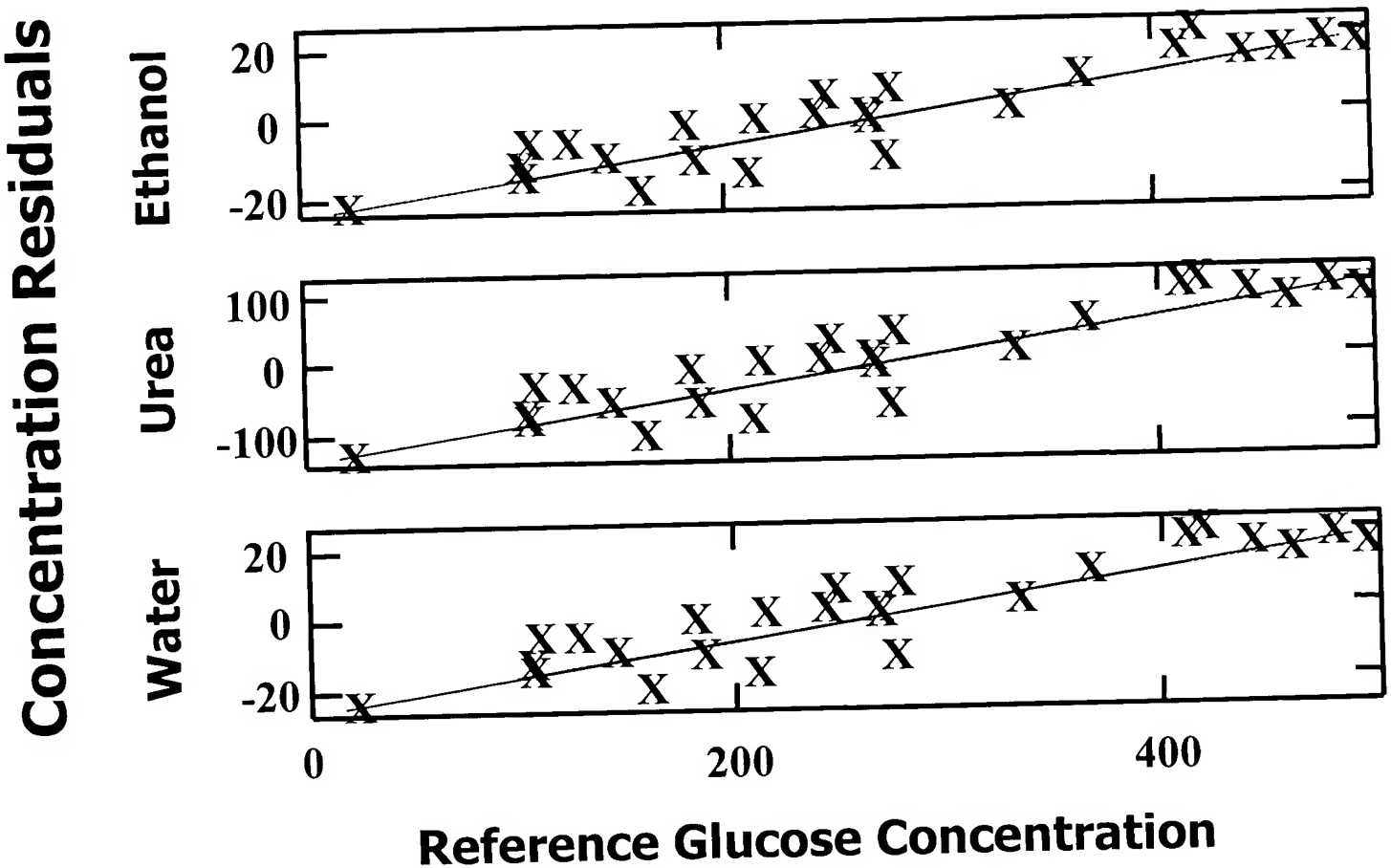


Fig. 10A

Fig. 10B

Fig. 10C

Augmented Alternating CLS

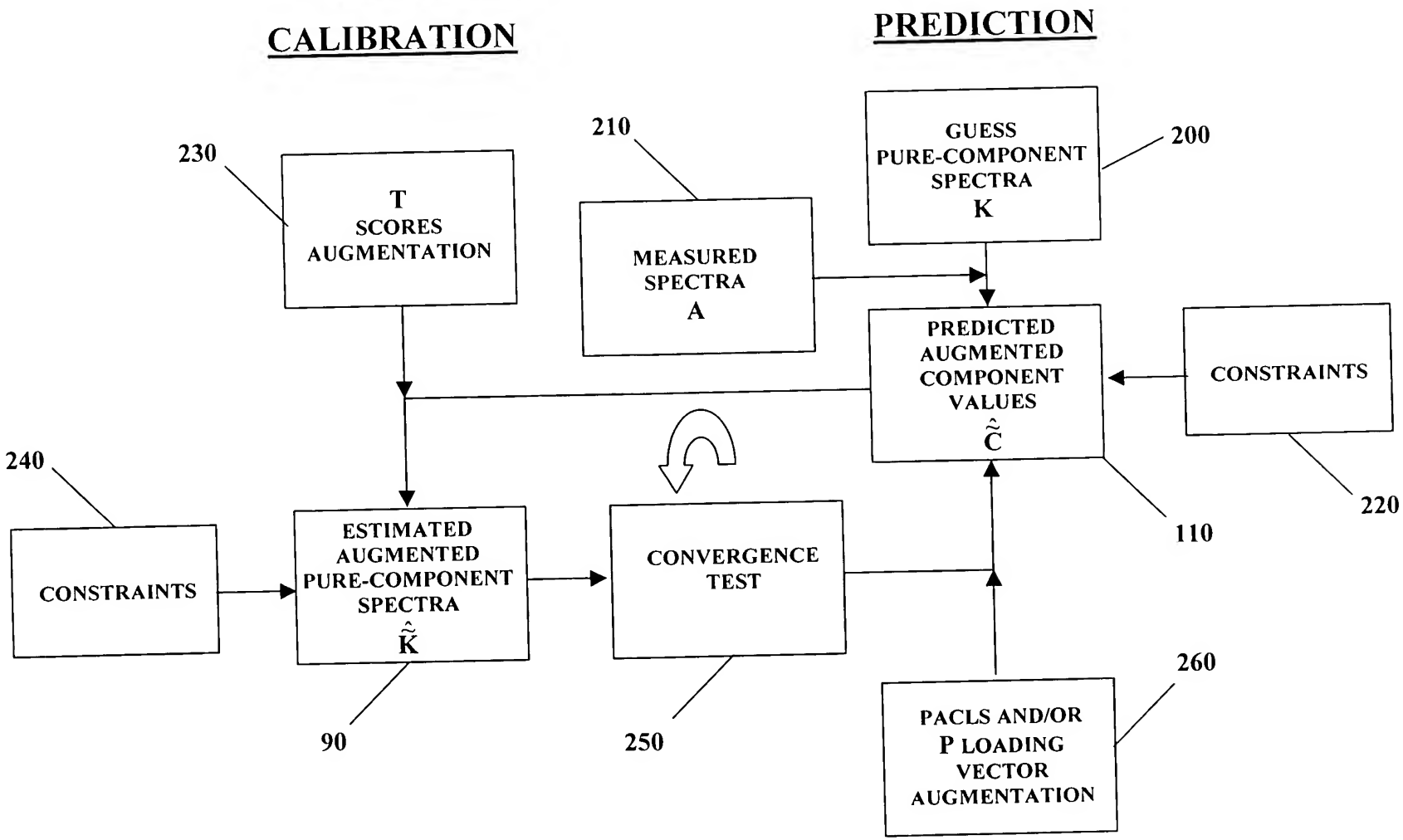


Fig. 11

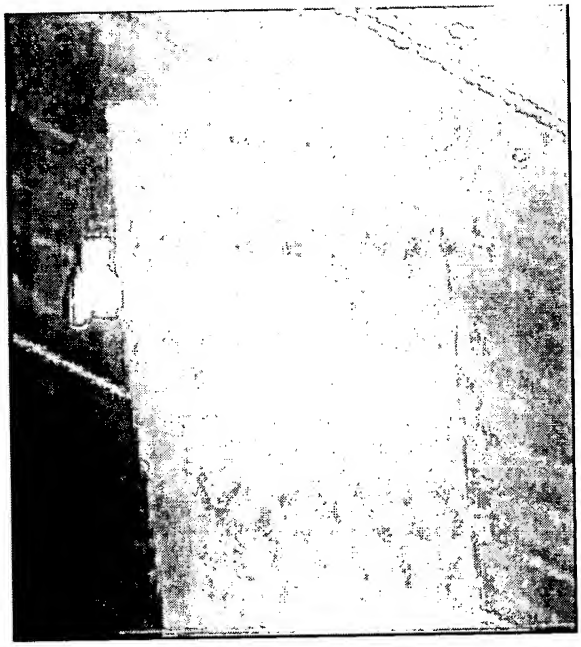


Fig. 12

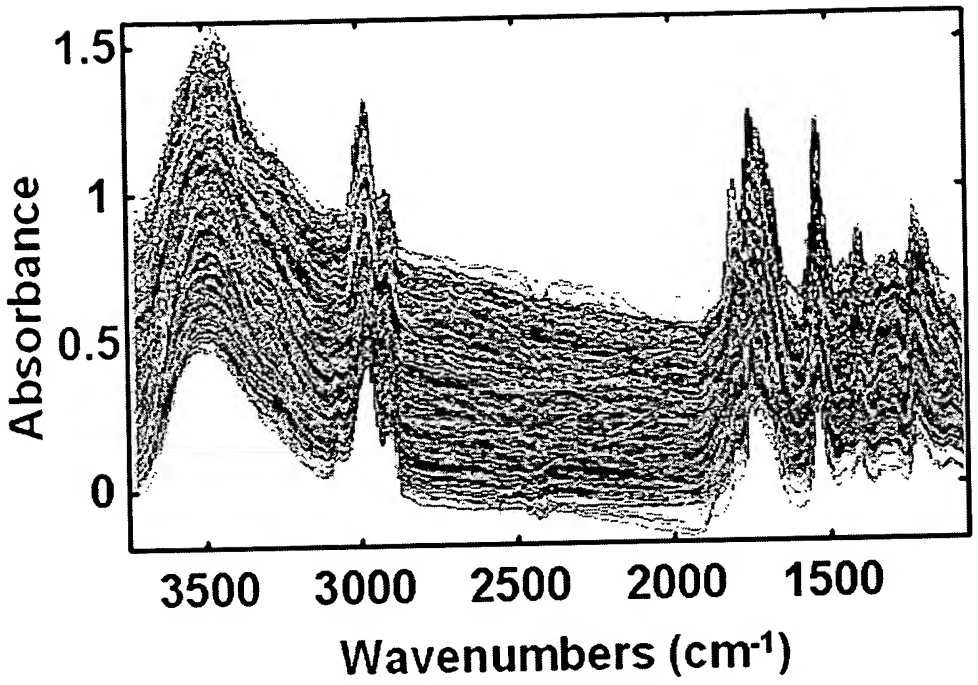


Fig. 13A

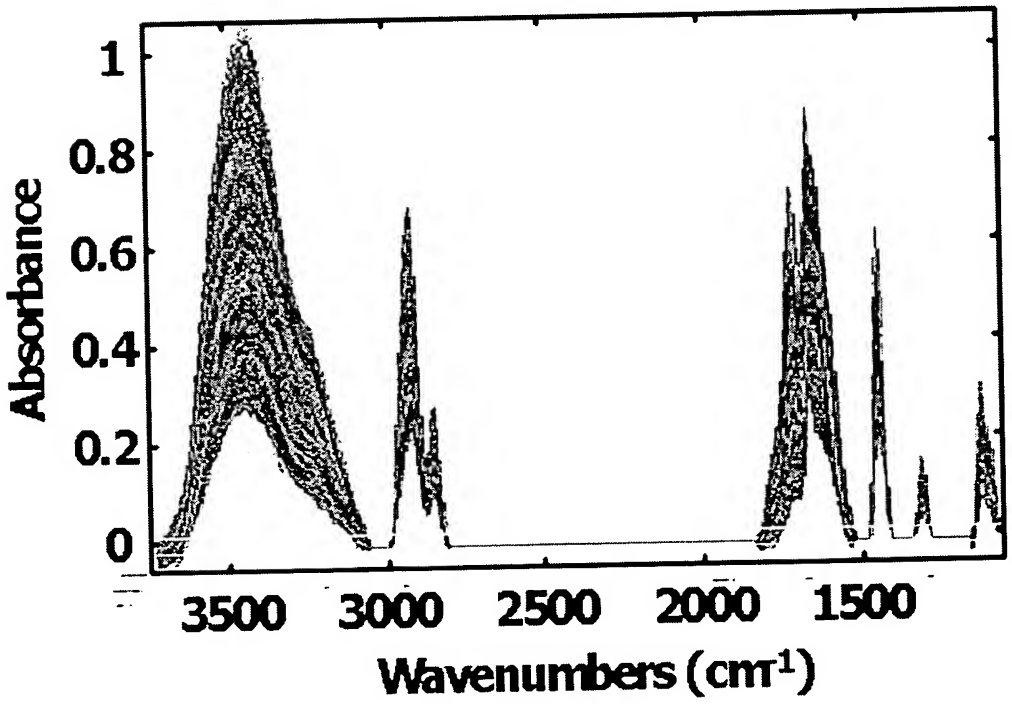


Fig. 13B

Fig. 14A

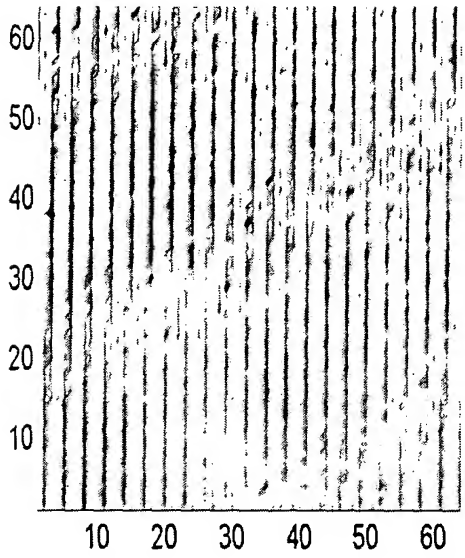


Fig. 14B

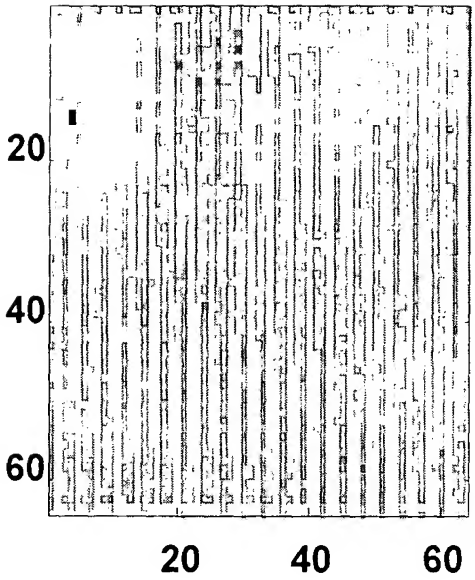


Fig. 14C

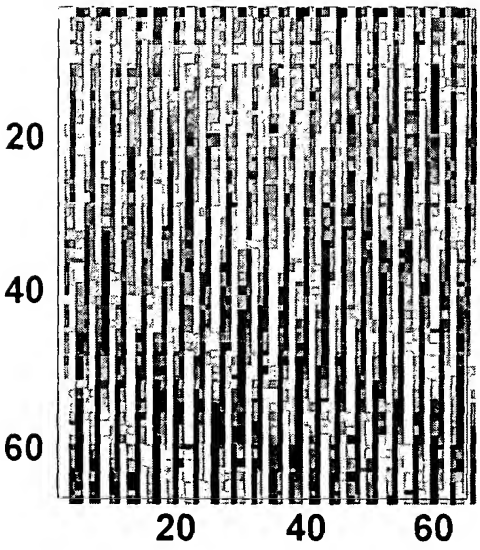
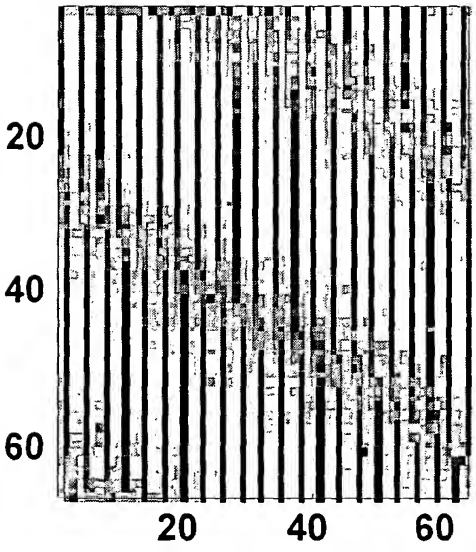



Fig. 14D